

Requester - Jan Heberle  
137653

Access DB# \_\_\_\_\_

## SEARCH REQUEST FORM

### Scientific and Technical Information Center

Requester's Full Name: Sabrina Cozzi Examiner #: 74141 Date: 11/12/09  
Art Unit: 1616 Phone Number (30) 206.22 Serial Number: 1613714  
Mail Box and Bldg/Room Location: 4C70, Rm, 4A45 Results Format Preferred (circle): PAPER  DISK  E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of invention: Therapeutic analogs  
Inventors (please provide full names): Corbett et al

Earliest Priority Filing Date: 7/3/2002

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Please search for compounds of Cls 12  
or 12 when A = C.

Please note 2 can be heterocyclic  
or amines acid, probably 2  
can be searched as N or Heterocyclic

Please see attached sheet

Thank you

STAFF USE ONLY		Type of Search	Vendors and cost where applicable
Searcher	<u>Jan</u>	NA Sequence (#)	STN <input checked="" type="checkbox"/>
Searcher Phone #	<u>22504</u>	AA Sequence (#)	Dialog
Searcher Location		Structure (#)	Questel/Orbit
Date Searcher Picked Up	<u>11/4</u>	Bibliographic	Dr Link
Date Compiled	<u>11/4</u>	Intaglio	Lexis/Nexis
Searcher Prep Review Time		Text	Sequence Systems
Critical Prep Time	<u>10</u>	Patent Family	WWW Internet
Review Time	<u>4:28</u>	Other	Other Specified

=> fil reg  
FILE 'REGISTRY' ENTERED AT 13:46:42 ON 14 NOV 2004  
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Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

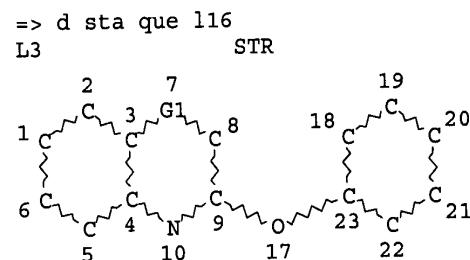
STRUCTURE FILE UPDATES: 12 NOV 2004 HIGHEST RN 780001-49-2  
DICTIONARY FILE UPDATES: 12 NOV 2004 HIGHEST RN 780001-49-2

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when  
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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

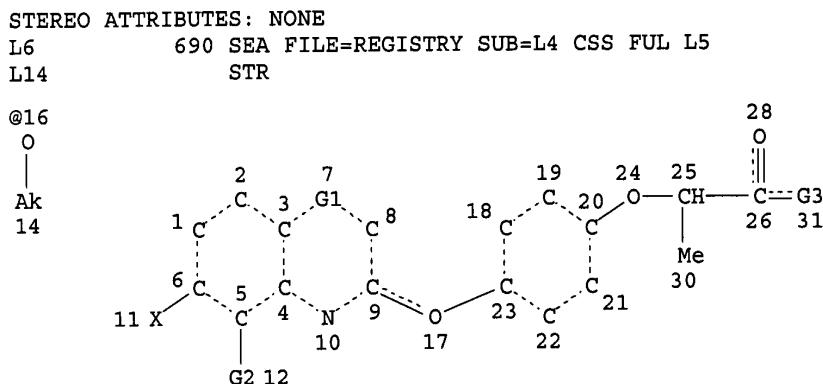


VAR G1=C/N  
NODE ATTRIBUTES:  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED  
  
GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE  
L4 ( 2621) SEA FILE=REGISTRY SSS FUL L3  
L5 STR

VAR G1=H/O/11  
NODE ATTRIBUTES:  
CONNECT IS M1 RC AT 7  
DEFAULT MLEVEL IS ATOM  
GGCAT IS PCY AT 2  
GGCAT IS MCY AT 4  
DEFAULT ECLEVEL IS LIMITED  
ECOUNT IS M1 N AT 2

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 11



VAR G1=C/N  
 VAR G2=H/OH/16  
 VAR G3=N/HY  
 NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE  
 L16 29 SEA FILE=REGISTRY SUB=L6 SSS FUL L14

100.0% PROCESSED 663 ITERATIONS 29 ANSWERS  
 SEARCH TIME: 00.00.01

=> d his 116-

(FILE 'REGISTRY' ENTERED AT 13:38:30 ON 14 NOV 2004)  
 L16 29 S L14 FUL SUB=L6  
 SAV L16 QAZI613C/A

FILE 'HCAPLUS' ENTERED AT 13:42:01 ON 14 NOV 2004  
 L17 5 S L16  
 L18 4 S L17 AND (HORWITZ J? OR CORBETT T? OR PALOMINO E? OR POLIN L?  
 L19 1 S L17 NOT L18  
 SEL RN L18

FILE 'REGISTRY' ENTERED AT 13:43:37 ON 14 NOV 2004  
 L20 189 S E1-E189  
 L21 59 S L20 AND L2 NOT L16  
 L22 2 S L21 AND C17H14CLN3O3  
 L23 1 S L22 NOT ALANINE  
 L24 30 S L16, L23  
 SAV L24 QAZI613D/A

FILE 'HCAOLD' ENTERED AT 13:46:15 ON 14 NOV 2004  
 L25 0 S L24

FILE 'HCAPLUS' ENTERED AT 13:46:17 ON 14 NOV 2004

L26 5 S L24

FILE 'USPATFULL' ENTERED AT 13:46:21 ON 14 NOV 2004  
 L27 2 S L24

FILE 'HCAPLUS' ENTERED AT 13:46:35 ON 14 NOV 2004  
 L28 5 S L26 AND L18-L19

FILE 'REGISTRY' ENTERED AT 13:46:42 ON 14 NOV 2004

=> fil uspatfull  
 FILE 'USPATFULL' ENTERED AT 13:46:55 ON 14 NOV 2004  
 CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 11 Nov 2004 (20041111/PD)  
 FILE LAST UPDATED: 11 Nov 2004 (20041111/ED)  
 HIGHEST GRANTED PATENT NUMBER: US6817028  
 HIGHEST APPLICATION PUBLICATION NUMBER: US2004226068  
 CA INDEXING IS CURRENT THROUGH 11 Nov 2004 (20041111/UPCA)  
 ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 11 Nov 2004 (20041111/PD)  
 REVISED CLASS FIELDS (/NCL) LAST RELOADED: Aug 2004  
 USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Aug 2004

>>> USPAT2 is now available. USPATFULL contains full text of the <<<  
 >>> original, i.e., the earliest published granted patents or <<<  
 >>> applications. USPAT2 contains full text of the latest US <<<  
 >>> publications, starting in 2001, for the inventions covered in <<<  
 >>> USPATFULL. A USPATFULL record contains not only the original <<<  
 >>> published document but also a list of any subsequent <<<  
 >>> publications. The publication number, patent kind code, and <<<  
 >>> publication date for all the US publications for an invention <<<  
 >>> are displayed in the PI (Patent Information) field of USPATFULL <<<  
 >>> records and may be searched in standard search fields, e.g., /PN, <<<  
 >>> /PK, etc. <<<

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 >>> through the new cluster USPATALL. Type FILE USPATALL to <<<  
 >>> enter this cluster. <<<  
 >>> <<<  
 >>> Use USPATALL when searching terms such as patent assignees, <<<  
 >>> classifications, or claims, that may potentially change from <<<  
 >>> the earliest to the latest publication. <<<

This file contains CAS Registry Numbers for easy and accurate  
 substance identification.

=> d 127 bib abs hitstr tot

L27 ANSWER 1 OF 2 USPATFULL on STN  
 AN 2004:172454 USPATFULL  
 TI Therapeutic amides  
 IN Horwitz, Jerome P., Farmington Hills, MI, UNITED STATES  
     Corbett, Thomas H., Grosse Pointe Park, MI, UNITED STATES  
     Palomino, Eduardo, Royal Oak, MI, UNITED STATES  
     Polin, Lisa, Oak Park, MI, UNITED STATES  
     Hazeldine, Stuart T., Taylor, MI, UNITED STATES  
 PI US 2004132618 A1 20040708  
 AI US 2003-613914 A1 20030703 (10)  
 PRAI US 2002-393858P 20020703 (60)  
 DT Utility  
 FS APPLICATION  
 LREP Schwegman, Lundberg, Woessner & Kluth, P.A., P.O. Box 2938, Minneapolis,  
     MN, 55402

CLMN Number of Claims: 64

ECL Exemplary Claim: 1

DRWN No Drawings

LN.CNT 2012

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention provides compounds of the formula: ##STR1##

wherein A, X, Y, and Z are as defined in the specification. The compounds are effective anti-tumor agents. The invention also provides pharmaceutical compositions comprising a compound of the above formula or a salt thereof, intermediates useful for preparing a compound of the above formula, and therapeutic methods comprising administering a compound of the above formula or a salt thereof to a mammal in need thereof.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 347162-71-4P 347162-73-6P 643752-97-0P

643752-98-1P 643753-00-8P 643753-02-0P

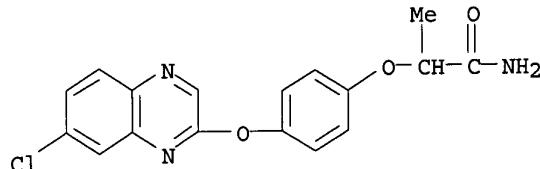
643753-03-1P 643753-05-3P 643753-06-4P

643753-11-1P 643753-12-2P 643753-13-3P

(preparation of therapeutic amides as antitumor agents)

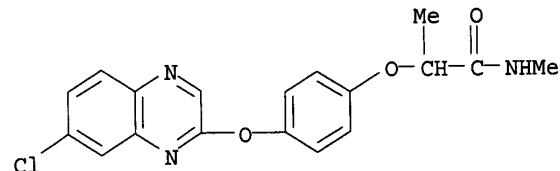
RN 347162-71-4 USPATFULL

CN Propanamide, 2-[4-[(7-chloro-2-quinoxalinyloxy]phenoxy]- (9CI) (CA INDEX NAME)



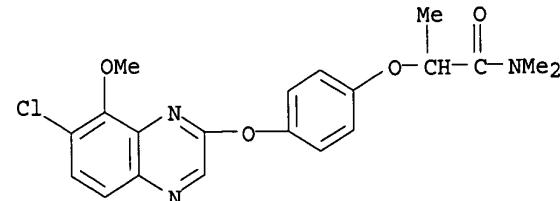
RN 347162-73-6 USPATFULL

CN Propanamide, 2-[4-[(7-chloro-2-quinoxalinyloxy]phenoxy]-N-methyl- (9CI) (CA INDEX NAME)

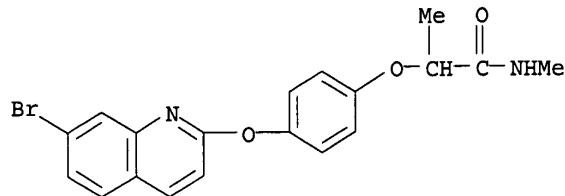


RN 643752-97-0 USPATFULL

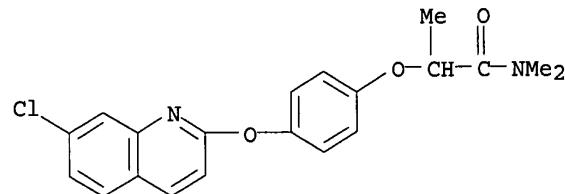
CN Propanamide, 2-[4-[(7-chloro-8-methoxy-2-quinoxalinyloxy]phenoxy]-N,N-dimethyl- (9CI) (CA INDEX NAME)



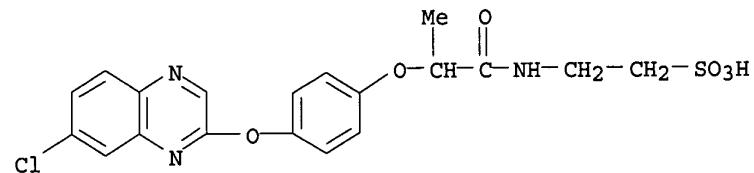
RN 643752-98-1 USPATFULL  
 CN Propanamide, 2-[4-[(7-bromo-2-quinolinyl)oxy]phenoxy]-N-methyl- (9CI) (CA INDEX NAME)



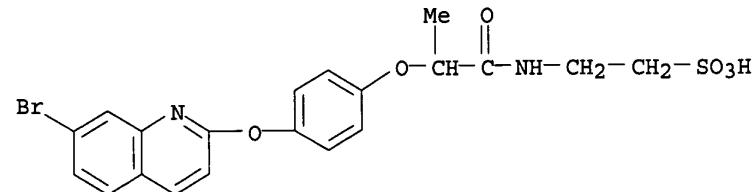
RN 643753-00-8 USPATFULL  
 CN Propanamide, 2-[4-[(7-chloro-2-quinolinyl)oxy]phenoxy]-N,N-dimethyl- (9CI) (CA INDEX NAME)



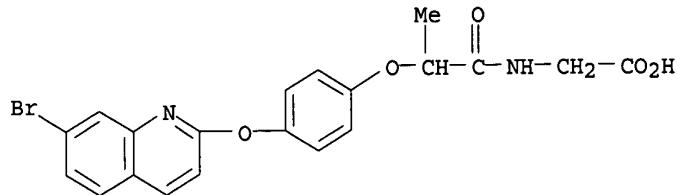
RN 643753-02-0 USPATFULL  
 CN Ethanesulfonic acid, 2-[[2-[4-[(7-chloro-2-quinolinalyl)oxy]phenoxy]-1-oxopropyl]amino]- (9CI) (CA INDEX NAME)



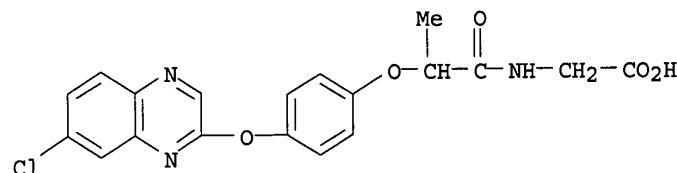
RN 643753-03-1 USPATFULL  
 CN Ethanesulfonic acid, 2-[[2-[4-[(7-bromo-2-quinolinyl)oxy]phenoxy]-1-oxopropyl]amino]- (9CI) (CA INDEX NAME)



RN 643753-05-3 USPATFULL  
 CN Glycine, N-[2-[4-[(7-bromo-2-quinolinyl)oxy]phenoxy]-1-oxopropyl]- (9CI) (CA INDEX NAME)

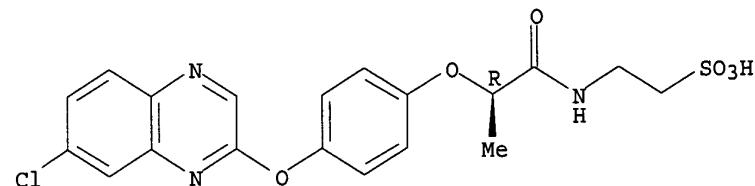


RN 643753-06-4 USPATFULL  
 CN Glycine, N-[2-[4-[(7-chloro-2-quinoxalinyl)oxy]phenoxy]-1-oxopropyl]-  
     (9CI) (CA INDEX NAME)

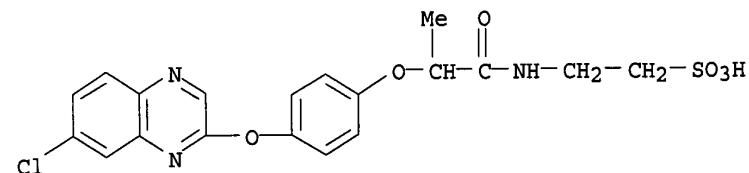


RN 643753-11-1 USPATFULL  
 CN Ethanesulfonic acid, 2-[(2R)-2-[4-[(7-chloro-2-quinoxalinyl)oxy]phenoxy]-  
     1-oxopropyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

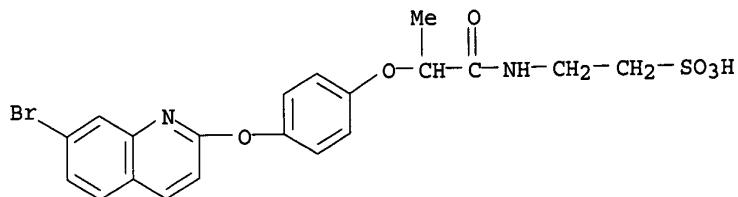


RN 643753-12-2 USPATFULL  
 CN Ethanesulfonic acid, 2-[(2-[(4-[(7-chloro-2-quinoxalinyl)oxy]phenoxy)-1-  
     oxopropyl]amino]-, monosodium salt (9CI) (CA INDEX NAME)



● Na

RN 643753-13-3 USPATFULL  
 CN Ethanesulfonic acid, 2-[(2-[(4-[(7-bromo-2-quinolinyl)oxy]phenoxy)-1-  
     oxopropyl]amino]-, monosodium salt (9CI) (CA INDEX NAME)

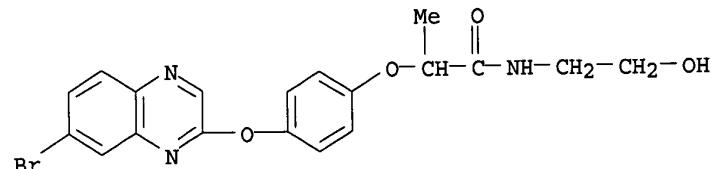


● Na

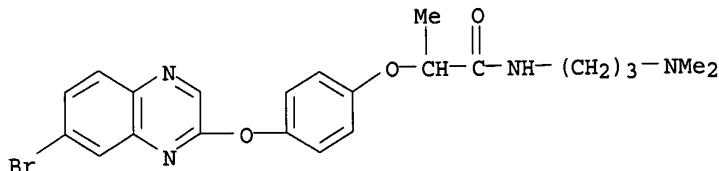
L27 ANSWER 2 OF 2 USPATFULL on STN  
 AN 97:115278 USPATFULL  
 TI (2-quinoxalinyloxy) phenoxypropanoic acids and related derivatives as  
 anticancer agents  
 IN Behrens, Carl Henry, Newark, DE, United States  
 Dusak, Betsy Ann, Secane, PA, United States  
 Harrison, Barbara Ann, Wilmington, DE, United States  
 Orwat, Michael James, Wilmington, DE, United States  
 PA The DuPont Merck Pharmaceutical Company, Wilmington, DE, United States  
 (U.S. corporation)  
 PI US 5696119 19971209  
 AI US 1994-367481 19941228 (8)  
 RLI Continuation of Ser. No. US 1992-991525, filed on 15 Dec 1992, now  
 abandoned  
 DT Utility  
 FS Granted  
 EXNAM Primary Examiner: Bernhardt, Emily  
 LREP Ferguson, Blair Q., Vance, David H.  
 CLMN Number of Claims: 20  
 ECL Exemplary Claim: 1  
 DRWN No Drawings  
 LN.CNT 1199  
 CAS INDEXING IS AVAILABLE FOR THIS PATENT.  
 AB This invention relates to (2-quinoxalinyloxy)phenoxypropanoic acids,  
 related derivatives thereof, enantiomeric and diastereomeric forms  
 thereof, mixtures of enantiomeric diastereomeric forms thereof, and  
 pharmaceutically acceptable salt forms thereof, pharmaceutical  
 compositions containing them, processes for their preparation, and  
 methods of using them to treat cancer, particularly solid tumors, in  
 mammals.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 157435-00-2P 157435-01-3P  
 (preparation of, as neoplasm inhibitor)  
 RN 157435-00-2 USPATFULL  
 CN Propanamide, 2-[4-[(7-bromo-2-quinoxalinyloxy)phenoxy]-N-(2-hydroxyethyl)-  
 (9CI) (CA INDEX NAME)



RN 157435-01-3 USPATFULL  
 CN Propanamide, 2-[4-[(7-bromo-2-quinoxalinyloxy]phenoxy]-N-[3-(dimethylamino)propyl]-(9CI) (CA INDEX NAME)



=> fil hcaplus  
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FILE COVERS 1907 - 14 Nov 2004 VOL 141 ISS 21  
 FILE LAST UPDATED: 12 Nov 2004 (20041112/ED)

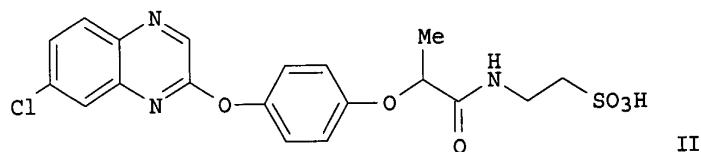
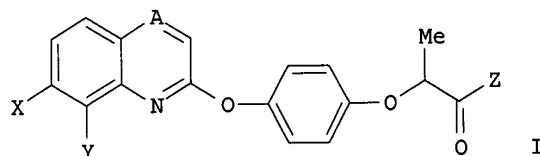
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d 128 all hitstr tot

L28 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2004:41446 HCAPLUS  
 DN 140:111288  
 ED Entered STN: 18 Jan 2004  
 TI Preparation of 2-[4-[(7-halo-2-quinolinyloxy]phenoxy]propionic acid derivatives and quinoxalinyloxy analogs as antineoplastic agents  
 IN Horwitz, Jerome P.; Corbett, Thomas H.; Palomino, Eduardo; Polin, Lisa; Hazeldine, Stuart T.  
 PA Wayne State University, USA  
 SO PCT Int. Appl., 67 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 IC ICM C07D215-22  
 ICS C07D241-44; A61K031-47; A61K031-498; A61P035-00  
 CC 27-17 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 1, 63  
 FAN.CNT 2  
 PATENT NO. KIND DATE APPLICATION NO. DATE  
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PI WO 2004005260 A1 20040115 WO 2003-US21062 20030703  
 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,  
 CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,  
 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,  
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,  
 PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,  
 TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,  
 KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,  
 FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,  
 BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG  
 US 2004132618 A1 20040708 US 2003-613914 20030703  
 PRAI US 2002-393858P P 20020703

CLASS		
PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2004005260	ICM	C07D215-22
	ICS	C07D241-44; A61K031-47; A61K031-498; A61P035-00
OS MARPAT 140:111288		
GI		



AB Title compds. I [wherein A = CH or N; X = F, Cl, or Br; Y = H, OH, or alkoxy; Z = an amino acid or heterocycle; and pharmaceutically acceptable salts thereof] were prepared and tested in vivo as antitumor agents. Preferred compds. of the invention and their pharmaceutical compns. are more potent and less toxic than the known antitumor agent, 2-[4-[(7-chloro-2-quinoxalinyloxy)phenoxy]propanoic acid sodium salt (XK 469), and have a different metabolic profile than XK 469. For example, XK 469 was refluxed with SOC12 for 1 h and the resulting acid chloride treated with  $\beta$ -aminoethylsulfonate (taurine) and 1M NaOH in THF to give II•Na (74%). Chiral HPLC separation afforded the enantiomers. (R)-II•Na was well tolerated in mice at a total dose of 1610 mg/kg i.v. and was highly active (T/C = 0%, log cell kill = 4.2) against early stage murine mammary adenocarcinoma 16/C. No adverse symptoms or cures were noted post injection.

ST quinolinylloxyphenoxy quinoxalinyloxyphenoxy propanoic acid prepn antitumor agent

IT Drug delivery systems  
 (aerosols; preparation of [[(haloquinolinyl)oxy]phenoxy]propionic acid derivs. and quinoxalinyloxyphenoxy propanoic acid derivs. and quinoxalinyloxyphenoxy propanoic acid as antineoplastic agents)

IT Drug delivery systems  
 (capsules; preparation of [[(haloquinolinyl)oxy]phenoxy]propionic acid derivs. and quinoxalinyloxyphenoxy propanoic acid as antineoplastic agents)

derivs. and quinoxalinyl analogs as antineoplastic agents)

IT Drug delivery systems  
(injections; preparation of [[(haloquinolinyloxy)phenoxy]propionic acid derivs. and quinoxalinyl analogs as antineoplastic agents)

IT Drug delivery systems  
(oral; preparation of [[(haloquinolinyloxy)phenoxy]propionic acid derivs. and quinoxalinyl analogs as antineoplastic agents)

IT Antitumor agents  
Human  
Neoplasm  
(preparation of [[(haloquinolinyloxy)phenoxy]propionic acid derivs. and quinoxalinyl analogs as antineoplastic agents)

IT Drug delivery systems  
(tablets; preparation of [[(haloquinolinyloxy)phenoxy]propionic acid derivs. and quinoxalinyl analogs as antineoplastic agents)

IT **643753-12-2P**  
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)  
(antitumor agent; preparation of [[(haloquinolinyloxy)phenoxy]propionic acid derivs. and quinoxalinyl analogs as antineoplastic agents)

IT **646505-47-7P 647026-59-3P**  
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(antitumor agent; preparation of [[(haloquinolinyloxy)phenoxy]propionic acid derivs. and quinoxalinyl analogs as antineoplastic agents)

IT **445041-69-0P**  
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(antitumor agent; preparation of [[(haloquinolinyloxy)phenoxy]propionic acid derivs. and quinoxalinyl analogs as antineoplastic agents)

IT **347162-71-4P 347162-73-6P 445041-75-8P,**  
(R)-2-[4-[(7-Bromo-2-quinolinyloxy)phenoxy]propionic acid  
**643752-97-0P 643753-00-8P, 2-[4-[(7-Chloro-2-**  
quinolinyloxy)phenoxy]-N,N-dimethylpropionamide **643753-13-3P**  
**646505-48-8P 646505-49-9P, (R)-[[2-[4-[(7-Bromoquinolin-2-yl)oxy]phenoxy]propionyl]amino]acetic acid 646505-50-2P,**  
(R)-[[2-[4-[(7-Chloroquinoxalin-2-yl)oxy]phenoxy]propionyl]amino]acetic acid **646505-51-3P**  
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(antitumor agent; preparation of [[(haloquinolinyloxy)phenoxy]propionic acid derivs. and quinoxalinyl analogs as antineoplastic agents)

IT **445041-74-7P, (R)-2-[4-[(7-Chloro-2-quinolinyloxy)phenoxy]propionic acid**  
**643752-98-1P, 2-[4-[(7-Bromo-2-quinolinyloxy)phenoxy]-N-**  
methylpropionamide **643753-02-0P 643753-03-1P**  
**643753-05-3P, [[2-[4-[(7-Bromoquinolin-2-yl)oxy]phenoxy]propionyl]amino]acetic acid 643753-06-4P,**  
[[2-[4-[(7-Chloroquinoxalin-2-yl)oxy]phenoxy]propionyl]amino]acetic acid **647026-61-7P**  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(antitumor agent; preparation of [[(haloquinolinyloxy)phenoxy]propionic acid derivs. and quinoxalinyl analogs as antineoplastic agents)

IT 56-40-6, Glycine, reactions 613-77-4, 2,7-Dichloroquinoline 7347-25-3  
94050-90-5, (R)-(+)-2-(4-Hydroxyphenoxy)propionic acid 99455-15-9,

7-Bromo-2-chloroquinoline 157434-99-6, XK 469 157542-89-7  
 157542-90-0 445041-70-3, 2-[4-[(7-Bromo-2-quinolinyl)oxy]phenoxy]propionic acid  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of [[(haloquinolinyl)oxy]phenoxy]propionic acid derivs. and  
 quinoxalinyln analogs as antineoplastic agents)

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

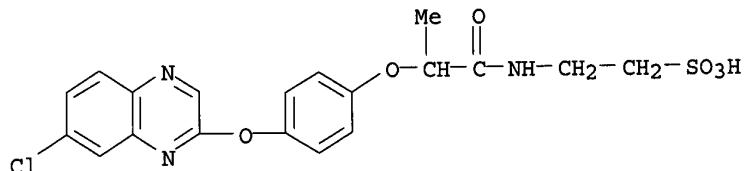
- (1) Corbett, T; INVESTIGATIONAL NEW DRUGS 1998, V16(2), P129 HCPLUS
- (2) Ikai, T; US 4629493 A 1986 HCPLUS
- (3) Stuart, H; J MED CHEM 2001, V44, P1758
- (4) Zi, K; US 6197728 B1 2001 HCPLUS

IT 643753-12-2P

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)  
 (antitumor agent; preparation of [[(haloquinolinyl)oxy]phenoxy]propionic acid derivs. and quinoxalinyln analogs as antineoplastic agents)

RN 643753-12-2 HCPLUS

CN Ethanesulfonic acid, 2-[[2-[4-[(7-chloro-2-quinoxalinyln)oxy]phenoxy]-1-oxopropyl]amino]-, monosodium salt (9CI) (CA INDEX NAME)



● Na

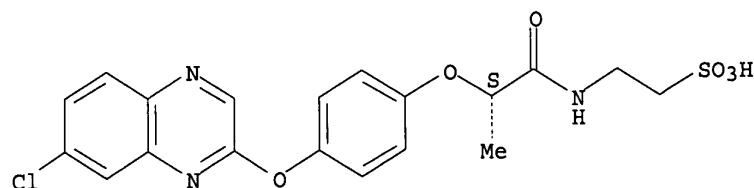
IT 646505-47-7P 647026-59-3P

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (antitumor agent; preparation of [[(haloquinolinyl)oxy]phenoxy]propionic acid derivs. and quinoxalinyln analogs as antineoplastic agents)

RN 646505-47-7 HCPLUS

CN Ethanesulfonic acid, 2-[[[(2S)-2-[4-[(7-chloro-2-quinoxalinyln)oxy]phenoxy]-1-oxopropyl]amino]-, monosodium salt (9CI) (CA INDEX NAME)

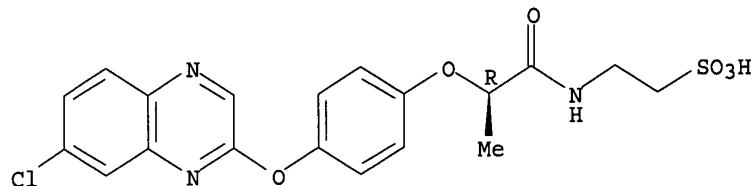
Absolute stereochemistry.



● Na

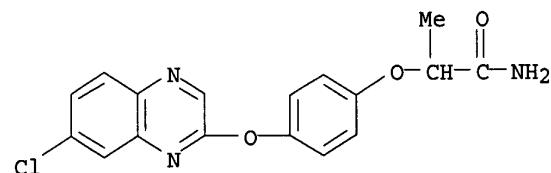
RN 647026-59-3 HCPLUS  
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Absolute stereochemistry. Rotation (+).

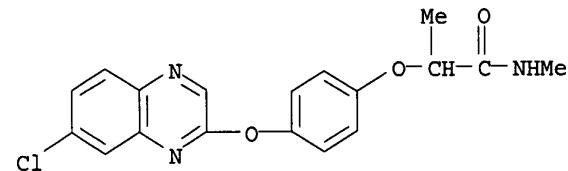


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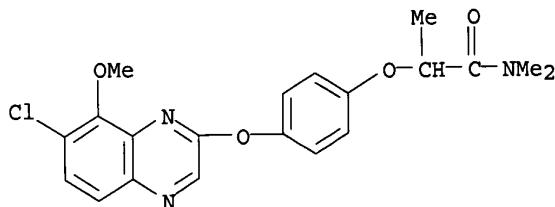
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 646505-49-9P, (R)-[2-[4-[(7-Bromoquinolin-2-yl)oxy]phenoxy]propionyl]amino]acetic acid 646505-50-2P,  
 (R)-[2-[4-[(7-Chloroquinoxalin-2-yl)oxy]phenoxy]propionyl]amino]acetic acid  
 RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (antitumor agent; preparation of [(haloquinolinyl)oxy]phenoxy]propionic acid derivs. and quinoxalinyl analogs as antineoplastic agents)  
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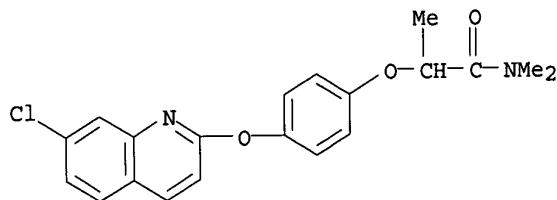
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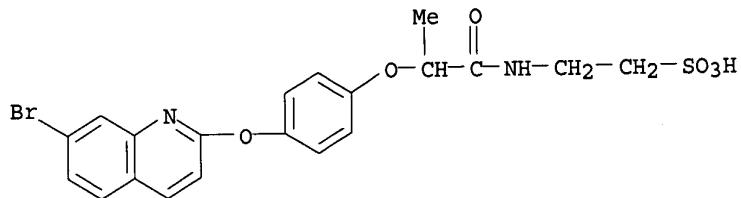
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RN 643753-00-8 HCAPLUS  
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 (CA INDEX NAME)



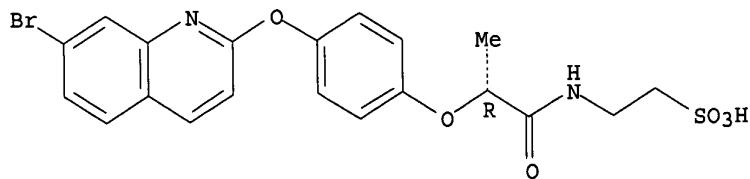
RN 643753-13-3 HCAPLUS  
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● Na

RN 646505-48-8 HCAPLUS  
 CN Ethanesulfonic acid, 2-[[2R)-2-[4-[(7-bromo-2-quinolinyloxy)phenoxy]-1-oxopropylamino]-, monosodium salt (9CI) (CA INDEX NAME)

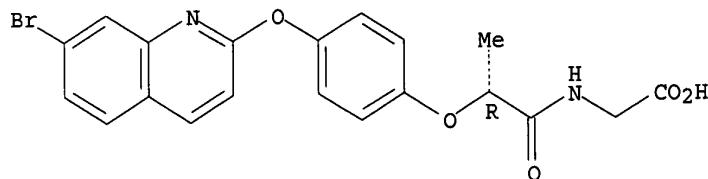
Absolute stereochemistry. Rotation (+).



● Na

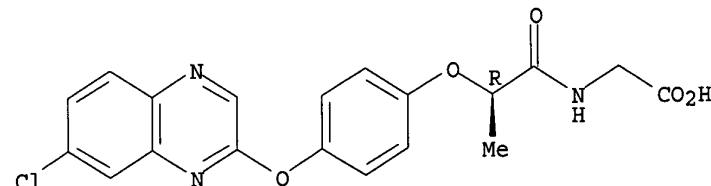
RN 646505-49-9 HCAPLUS  
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 (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

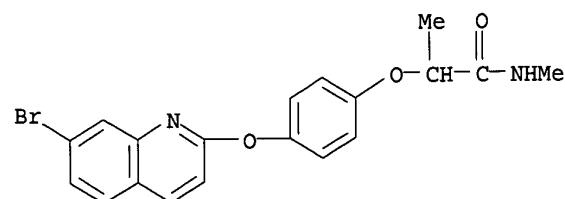


RN 646505-50-2 HCAPLUS  
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 (9CI) (CA INDEX NAME)

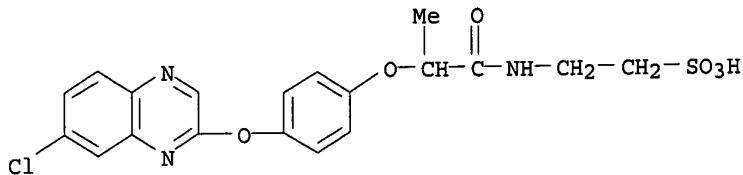
Absolute stereochemistry. Rotation (+).



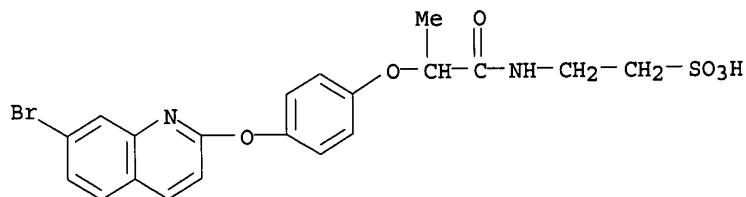
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 643753-05-3P, [[2-[4-[(7-Bromoquinolin-2-yl)oxy]phenoxy]propionyl]amino]acetic acid 643753-06-4P,  
 [[2-[4-[(7-Chloroquinoxalin-2-yl)oxy]phenoxy]propionyl]amino]acetic acid 647026-61-7P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)  
 (antitumor agent; preparation of [[(haloquinolinyl)oxy]phenoxy]propionic  
 acid derivs. and quinoxalinyl analogs as antineoplastic agents)  
 RN 643752-98-1 HCAPLUS  
 CN Propanamide, 2-[4-[(7-bromo-2-quinolinyl)oxy]phenoxy]-N-methyl- (9CI) (CA INDEX NAME)



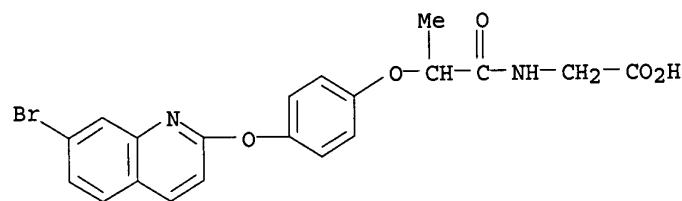
RN 643753-02-0 HCAPLUS  
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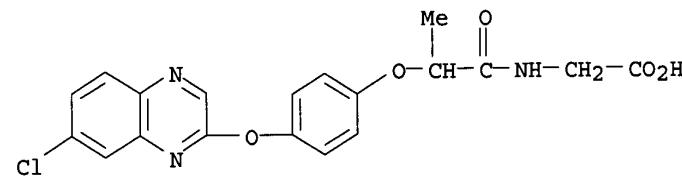
RN 643753-03-1 HCAPLUS  
 CN Ethanesulfonic acid, 2-[[2-[4-[(7-bromo-2-quinolinyloxy)phenoxy]-1-oxopropyl]amino]- (9CI) (CA INDEX NAME)



RN 643753-05-3 HCAPLUS  
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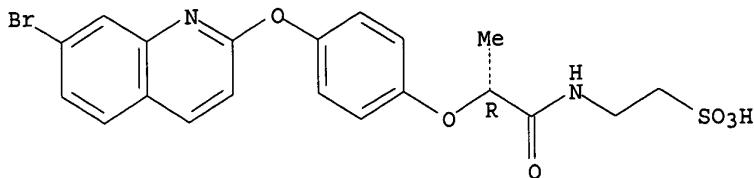


RN 643753-06-4 HCAPLUS  
 CN Glycine, N-[2-[(4-[(7-chloro-2-quinolinyloxy)phenoxy]-1-oxopropyl]- (9CI) (CA INDEX NAME)



RN 647026-61-7 HCAPLUS  
 CN Ethanesulfonic acid, 2-[[2R)-2-[4-[(7-bromo-2-quinolinyloxy)phenoxy]-1-oxopropyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L28 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2004:41220 HCAPLUS

DN 140:99632

ED Entered STN: 18 Jan 2004

TI Preparation of therapeutic amides as antitumor agents

IN Horwitz, Jerome P.; Corbett, Thomas H.; Palomino, Eduardo; Polin, Lisa; Hazeldine, Stuart T.

PA Wayne State University, USA

SO PCT Int. Appl., 52 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM A61K

CC 63-6 (Pharmaceuticals)

Section cross-reference(s): 1, 28

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004004651	A2	20040115	WO 2003-US21126	20030703
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2004132618	A1	20040708	US 2003-613914	20030703
PRAI	US 2002-393858P	P	20020703		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2004004651	ICM	A61K

OS MARPAT 140:99632

AB Amides, e.g., 2-[4-((7-bromo-2-quinolinyloxy)phenoxy)propionylmethylamide, {2-[4-(7-bromoquinolin-2-yl)phenoxy]propionylamino}acetic acid, or {2-[4-(7-chloro-2-quinolinyloxy)phenoxy]propionylaminoethanesulfonic acid, are prepared for use as effective antitumor agents. The invention also provides pharmaceutical compns. comprising the above compound, intermediates useful for preparing the compds., and methods for administering the compds. to a mammal. Thus, sodium (2-(4-(7-chloro-2-quinolinyloxy)phenoxy)propionylaminoethanesulfonate was prepared in a series of steps by starting from Et vinyl ether with oxalyl chloride followed by treatment with substituted anilines cyclization, and subsequent treatment with 2-(4-hydroxyphenoxy)propionic acid. Tablets contained the above compound 100.0, lactose 77.5, Povidone 15.0, Croscarmellose sodium 12.0, microcryst. cellulose 92.5, and Mg stearate 3.0 mg/tablet. The compound had activity against adenocarcinoma.

ST therapeutic amide antitumor prep

IT Carcinoma

(adenocarcinoma; preparation of therapeutic amides as antitumor agents)

IT Drug delivery systems  
(aerosols; preparation of therapeutic amides as antitumor agents)

IT Drug delivery systems  
(capsules; preparation of therapeutic amides as antitumor agents)

IT Drug delivery systems  
(injections; preparation of therapeutic amides as antitumor agents)

IT Antitumor agents  
Neoplasm  
(preparation of therapeutic amides as antitumor agents)

IT Amides, biological studies  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of therapeutic amides as antitumor agents)

IT Drug delivery systems  
(tablets; preparation of therapeutic amides as antitumor agents)

IT 23952-31-0P 59412-12-3P 99455-13-7P 160893-07-2P 455955-27-8P  
RL: BYP (Byproduct); PREP (Preparation)  
(preparation of therapeutic amides as antitumor agents)

IT 347162-71-4P 347162-73-6P 643752-97-0P  
643752-98-1P 643753-00-8P 643753-02-0P  
643753-03-1P 643753-05-3P 643753-06-4P  
643753-11-1P 643753-12-2P 643753-13-3P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of therapeutic amides as antitumor agents)

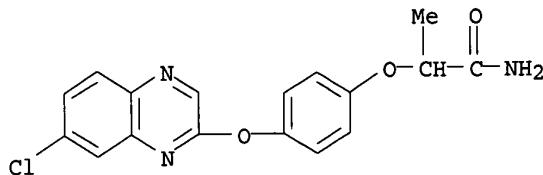
IT 56-40-6, Glycine, reactions 79-37-8, Oxalyl chloride 107-35-7, Taurine 108-42-9 108-44-1, reactions 109-92-2, Ethyl vinyl ether 372-19-0 536-90-3 591-19-5 67648-61-7 94050-90-5 99471-66-6, trans-3-Ethoxyacryloyl chloride  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of therapeutic amides as antitumor agents)

IT 613-77-4P 4053-33-2P 4053-35-4P 4295-12-9P 22614-72-8P  
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of therapeutic amides as antitumor agents)

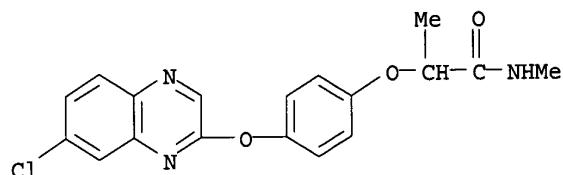
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of therapeutic amides as antitumor agents)

RN 347162-71-4 HCPLUS

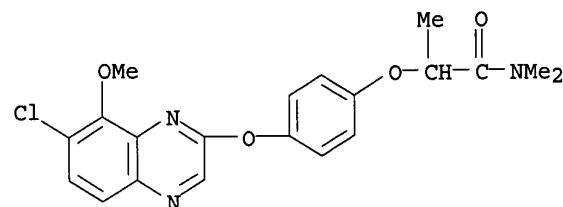
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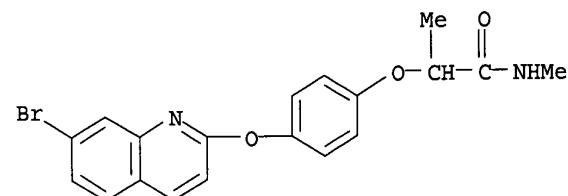
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 (CA INDEX NAME)



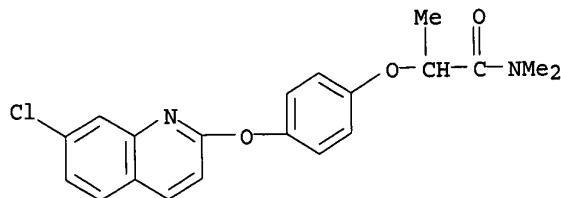
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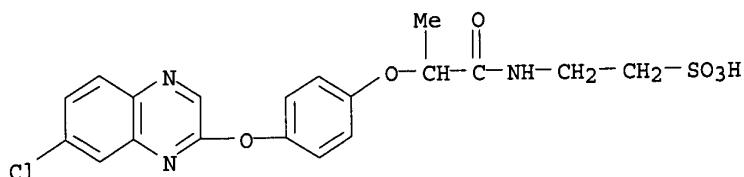
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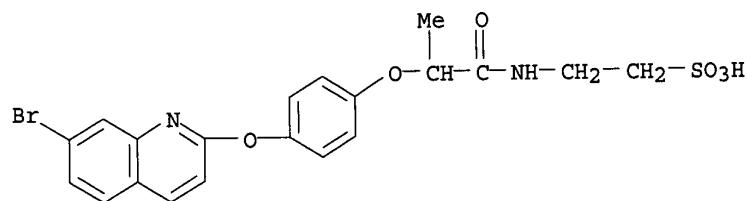
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 (CA INDEX NAME)



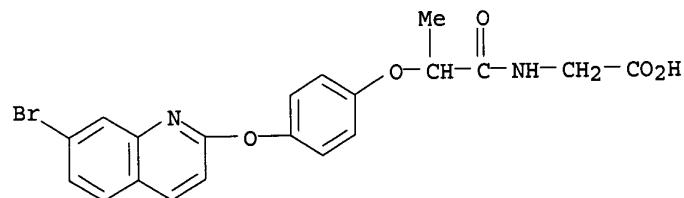
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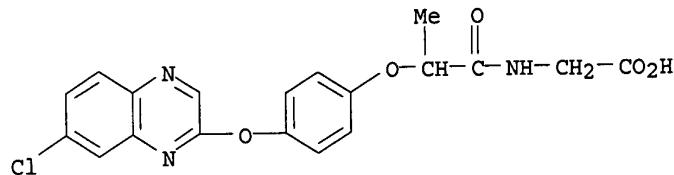
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 CN Ethanesulfonic acid, 2-[[2-[4-[(7-bromo-2-quinolinyloxy)phenoxy]-1-oxopropyl]amino]- (9CI) (CA INDEX NAME)



RN 643753-05-3 HCAPLUS  
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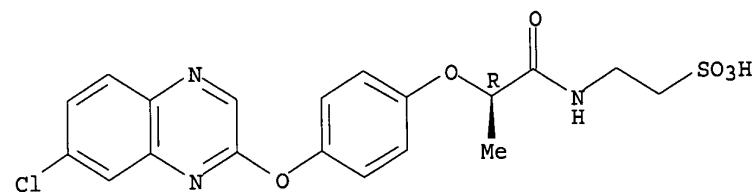


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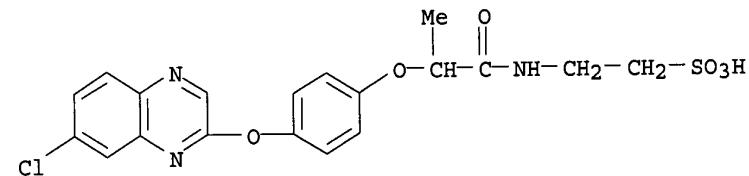


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Absolute stereochemistry. Rotation (+).

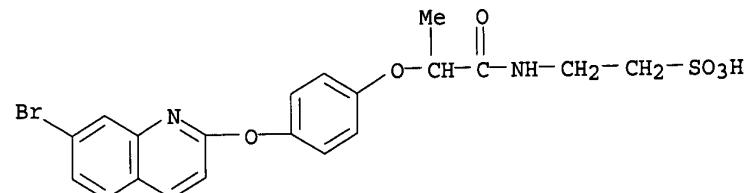


RN 643753-12-2 HCPLUS  
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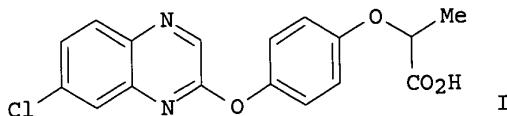
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RN 643753-13-3 HCPLUS  
 CN Ethanesulfonic acid, 2-[(2-[(4-[(7-bromo-2-quinolinyloxy)phenoxy]1-oxopropyl)amino]-1-oxopropyl)amino]-, monosodium salt (9CI) (CA INDEX NAME)



● Na

L28 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2001:301100 HCAPLUS  
 DN 135:76849  
 ED Entered STN: 29 Apr 2001  
 TI Design, Synthesis, and Biological Evaluation of Analogues of the Antitumor Agent, 2-{4-[(7-Chloro-2-quinoxalinyloxy)phenoxy}propionic Acid (XK469)  
 AU Hazeldine, Stuart T.; Polin, Lisa; Kushner, Juwanna; Paluch, Jennifer; White, Kathryn; Edelstein, Matthew; Palomino, Eduardo; Corbett, Thomas H.; Horwitz, Jerome P.  
 CS Department of Internal Medicine Division of Hematology and Oncology, Wayne State University School of Medicine, Detroit, MI, 48201, USA  
 SO Journal of Medicinal Chemistry (2001), 44(11), 1758-1776  
 CODEN: JMCMAR; ISSN: 0022-2623  
 PB American Chemical Society  
 DT Journal  
 LA English  
 CC 28-18 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1  
 OS CASREACT 135:76849  
 GI



AB 2-{4-[(7-Chloro-2-quinoxalinyloxy)phenoxy}propionic acid (XK469) I is among the most highly and broadly active antitumor agents to have been evaluated and scheduled to enter clin. trials in 2001. The mechanism or mechanisms of action of I remain to be elaborated. Accordingly, an effort was initiated to establish a pharmacophore hypothesis to delineate the requirements of the active site, via a comprehensive program of synthesis of analogs of I and evaluation of the effects of structural modification(s) on solid tumor activity. The strategy formulated chose to dissect the two-dimensional parent structure into three regions: I, ring A of quinoxaline; II, the hydroquinone connector linkage; and III, the lactic acid moiety-to determine the resultant in vitro and in vivo effects of chemical alterations in each region. Neither the A-ring unsubstituted nor the B-ring 3-chloro-regioisomer of I showed antitumor activity. The modulating antitumor effect(s) of substituents of differing

electronegativities, located at the several sites comprising the A-ring of region I, were next ascertained. Thus, a halogen substituent, located at the 7-position of a 2-{4-[(2-quinoxalinyloxy)phenoxy}propionic acid, generated the most highly and broadly active antitumor agents. A Me, methoxy, or an azido substituent at this site generated a much less active structure, whereas 5-, 6-, 8-chloro-, 6-, 7-nitro, and 7-amino derivs. all proved to be essentially inactive. When the connector linkage (region II) of I was changed from that of a hydroquinone to either a resorcinol or a catechol derivative, all antitumor activity was lost. Of the carboxylic acid derivs. of I (region III), i.e., CONH<sub>2</sub>, CONHMe, CONMe<sub>2</sub>, CONHOH, CONHNH<sub>2</sub>, CN, or CN<sub>4</sub>H (tetrazole), only the monomethyl- and N,N-dimethylamides proved to be active.

ST chloroquinoxalinyloxyphenoxypropionic acid structure antitumor; quinoxalinyloxyphenoxypropionic acid antitumor prep

IT Structure-activity relationship  
 (antitumor; preparation of antitumor (chloroquinoxalinyloxy)phenoxypropionic acid analogs from (chloro)quinoxalonols)

IT Antitumor agents  
 (preparation of antitumor (chloroquinoxalinyloxy)phenoxypropionic acid analogs from (chloro)quinoxalonols)

IT 347162-49-6P  
 RL: BYP (Byproduct); PREP (Preparation)  
 (formation of (oxoquinoxalinyl)propionate byproduct in preparation of  
 antitumor (chloroquinoxalinyl)propionic acid from  
 chloroquinoxalinols)

IT 347162-28-1P 347162-30-5P 347162-32-7P 347162-34-9P 347162-36-1P  
 347162-37-2P 347162-39-4P 347162-41-8P 347162-43-0P 347162-45-2P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
 study, unclassified); SPN (Synthetic preparation); BIOL (Biological  
 study); PREP (Preparation)  
 (preparation and structure-activity study of antitumor  
 (chloroquinoxalinyl)phenoxypropionic acid analogs)

IT 106744-85-8P 347162-29-2P 347162-31-6P 347162-33-8P 347162-35-0P  
 347162-38-3P 347162-40-7P 347162-42-9P 347162-44-1P 347162-46-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and structure-activity study of antitumor  
 (chloroquinoxalinyl)phenoxypropionic acid analogs)

IT 60075-04-9, Methyl 2-(4-hydroxyphenoxy)propionate  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of (chloroquinoxalinyl)phenoxypropionic acid analogs from  
 chloroquinoxalinols as antitumor agents)

IT 347162-27-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation of (chloroquinoxalinyl)phenoxypropionic acid analogs from  
 chloroquinoxalinols as antitumor agents)

IT 123-30-8, 4-Hydroxyaniline 535-11-5, Ethyl 2-bromopropionate  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of (phenylamino)propionate in synthesis of antitumor  
 (chloroquinoxalinyl)phenoxypropionic acid analogs)

IT 35897-44-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation of (phenylamino)propionate in synthesis of antitumor  
 (chloroquinoxalinyl)phenoxypropionic acid analogs)

IT 637-89-8, 4-Mercaptophenol  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of (phenylthiopropionate) in synthesis of antitumor  
 (chloroquinoxalinyl)phenoxypropionic acid analogs)

IT 347162-60-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation of (phenylthiopropionate) in synthesis of antitumor  
 (chloroquinoxalinyl)phenoxypropionic acid analogs)

IT 220935-29-5P 347162-54-3P 347162-62-3P 347162-64-5P  
 347162-71-4P 347162-72-5P 347162-73-6P  
 347162-76-9P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
 study, unclassified); SPN (Synthetic preparation); BIOL (Biological  
 study); PREP (Preparation)  
 (preparation of antitumor (chloroquinoxalinyl)phenoxypropionic acid  
 analogs)

IT 21023-20-1 78104-71-9 157435-10-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of antitumor (chloroquinoxalinyl)phenoxypropionic acid  
 analogs)

IT 347162-53-2P 347162-55-4P 347162-57-6P 347162-61-2P 347162-63-4P  
 347162-65-6P 347162-66-7P 347162-68-9P 347162-69-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation of antitumor (chloroquinoxalinyl)phenoxypropionic acid  
 analogs)

IT 5445-17-0, Methyl 2-bromopropionate 59489-30-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of antitumor (chloroquinoxalinyloxy)propionic acid from chloroquinoxalinols)

IT 347162-48-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of antitumor (chloroquinoxalinyloxy)propionic acid from chloroquinoxalinols)

IT 769-11-9, 2-Chloro-6-nitroaniline 59483-54-4, 3-Chloro-2-nitroaniline 89793-13-5 89975-38-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of chloroquinoxalines from (chloro)nitroanilines in synthesis of (chloroquinoxalinyloxy)phenoxypropionic acid analogs as antitumor agents)

IT 55687-05-3P, 2,5-Dichloroquinoxaline 55687-19-9P 65180-12-3P  
 120258-69-7P 347162-12-3P 347162-13-4P 347162-14-5P 347162-19-0P  
 347162-20-3P 347162-21-4P 347162-22-5P 347162-23-6P 347162-24-7P  
 347162-25-8P 347162-26-9P 347162-92-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of chloroquinoxalines from (chloro)nitroanilines in synthesis of (chloroquinoxalinyloxy)phenoxypropionic acid analogs as antitumor agents)

IT 20691-72-9, 4-Iodo-2-nitroaniline  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of chloroquinoxalines from nitroanilines in synthesis of (chloroquinoxalinyloxy)phenoxypropionic acid analogs as antitumor agents)

IT 55686-93-6P, 2-Chloro-7-methoxyquinoxaline 59489-31-5P,  
 2,7-Dichloroquinoxaline 90272-84-7P 347162-15-6P 347162-16-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of chloroquinoxalines from nitroanilines in synthesis of (chloroquinoxalinyloxy)phenoxypropionic acid analogs as antitumor agents)

IT 25652-34-0 55687-28-0 62573-36-8 66367-04-2 89898-96-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of chloroquinoxalines from nitroanilines in synthesis of antitumor (chloroquinoxalinyloxy)phenoxypropionic acid)

IT 347162-77-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of chloroquinoxalines from nitroanilines in synthesis of antitumor (chloroquinoxalinyloxy)phenoxypropionic acid analogs)

IT 98555-00-1  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of chloroquinoxalines from quinoxalinols in synthesis of (chloroquinoxalinyloxy)phenoxypropionic acid analogs as antitumor agents)

IT 6272-25-9P, 2-Chloro-6-nitroquinoxaline 55686-94-7P,  
 2-Chloro-7-nitroquinoxaline 347162-17-8P 347162-18-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of chloroquinoxalines from quinoxalinols in synthesis of (chloroquinoxalinyloxy)phenoxypropionic acid analogs as antitumor agents)

IT 347162-75-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of inactive antitumor (chloroquinoxalinyloxy)phenoxypropionic acid analogs)

IT 347162-47-4P 347162-56-5P 347162-58-7P 347162-67-8P 347162-70-3P

347162-74-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of inactive antitumor (chloroquinoxalinyloxy)phenoxypropionic acid analogs)

IT 347162-50-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of inactive antitumor (chloroquinoxalinyloxy)propionic acid from chloroquinoxalinols)

IT 92-88-6, 4,4'-Dihydroxybiphenyl 108-46-3, 1,3-Dihydroxybenzene, reactions 6272-38-4, 2-(Benzylxy)phenol  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of phenoxypropionates in synthesis of antitumor (chloroquinoxalinyloxy)phenoxypropionic acid analogs)

IT 87129-34-8P, Methyl 2-(3-hydroxyphenoxy)propionate 138426-35-4P  
 347162-51-0P 347162-52-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of phenoxypropionates in synthesis of antitumor (chloroquinoxalinyloxy)phenoxypropionic acid analogs)

IT 103-16-2, 4-(Benzylxy)phenol  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of phenoxypropionitrile in synthesis of antitumor (chloroquinoxalinyloxy)phenoxypropionic acid analogs)

IT 23194-54-9P 343866-65-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of phenoxypropionitrile in synthesis of antitumor (chloroquinoxalinyloxy)phenoxypropionic acid analogs)

RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD

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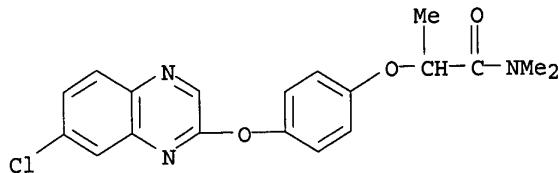
IT 220935-29-5P 347162-71-4P 347162-72-5P

347162-73-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (preparation of antitumor (chloroquinoxalinyloxy)phenoxypropionic acid analogs)

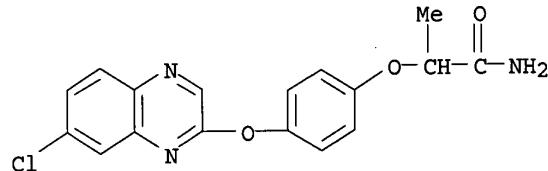
RN 220935-29-5 HCPLUS

CN Propanamide, 2-[4-[(7-chloro-2-quinoxalinyloxy)phenoxy]-N,N-dimethyl- (9CI) (CA INDEX NAME)



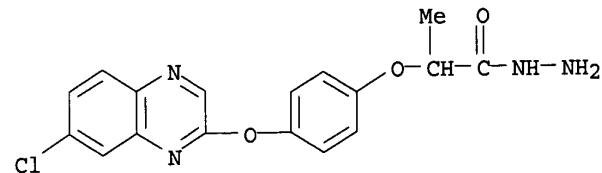
RN 347162-71-4 HCPLUS

CN Propanamide, 2-[4-[(7-chloro-2-quinoxalinyloxy)phenoxy]- (9CI) (CA INDEX NAME)



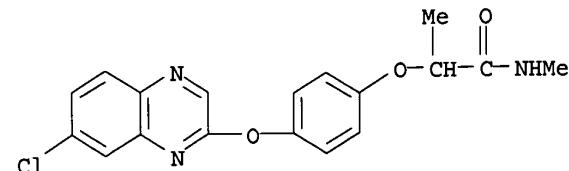
RN 347162-72-5 HCPLUS

CN Propanoic acid, 2-[4-[(7-chloro-2-quinoxalinyloxy)phenoxy]-, hydrazide (9CI) (CA INDEX NAME)

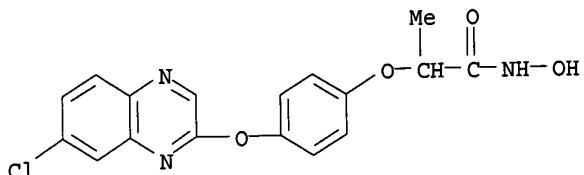


RN 347162-73-6 HCPLUS

CN Propanamide, 2-[4-[(7-chloro-2-quinoxalinyloxy)phenoxy]-N-methyl- (9CI) (CA INDEX NAME)



IT 347162-74-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of inactive antitumor (chloroquinoxalinyloxy)phenoxypropionic  
 acid analogs)  
 RN 347162-74-7 HCAPLUS  
 CN Propanamide, 2-[4-[(7-chloro-2-quinoxalinyloxy)phenoxy]-N-hydroxy- (9CI)  
 (CA INDEX NAME)



L28 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1998:787599 HCAPLUS  
 DN 130:204665  
 ED Entered STN: 16 Dec 1998  
 TI Preclinical antitumor efficacy of analogs of XK469: sodium-(2-[4-(7-chloro-2-quinoxalinyloxy)phenoxy]propionate)  
 AU Corbett, Thomas H.; LoRusso, Patricia; Demchick, Lisa; Simpson, Chiab; Pugh, Susan; White, Kathryn; Kushner, Juiwanna; Polin, Lisa; Meyer, Jennifer; Czarnecki, Jennifer; Heilbrun, Lance; Horwitz, Jerome P.; Gross, Janet L.; Behrens, Carl H.; Harrison, Barbara A.; McRipley, Ron J.; Trainor, George  
 CS School of Medicine, Wayne State University, Detroit, USA  
 SO Investigational New Drugs (1998), 16(2), 129-139  
 CODEN: INNDDK; ISSN: 0167-6997  
 PB Kluwer Academic Publishers  
 DT Journal  
 LA English  
 CC 1-3 (Pharmacology)  
 AB A series of quinoxaline analogs of the herbicide Assure was found to have selective cytotoxicity for solid tumors of mice in a disk-diffusion-soft-agar-colony-formation-assay compared to L1210 leukemia. Four agents without selective cytotoxicity and 14 agents with selective cytotoxicity were evaluated in vivo for activity against a solid tumor. The four agents without selective cytotoxicity in the disk-assay were inactive in vivo (T/C > 42%). Thirteen of the fourteen agents with selectivity in the disk-assay were active in vivo (T/C < 42%). Five of the agents had curative activity. These five agents had a halogen (F, Cl, Br) in the 7-position (whereas Assure had a Cl in the 6 position). All agents with curative activity were either a carboxylic acid, or a derivative thereof, whereas Assure is the Et ester of the carboxylic acid. All other structural features were identical between Assure and the curative agents. Assure had no selective cytotoxicity for solid tumors in the disk-assay, and was devoid of antitumor activity. The analog XK469 is in clin. development.  
 ST Assure quinoxaline analog antitumor structure  
 IT Structure-activity relationship  
 (antitumor; preclin. antitumor efficacy of quinoxaline analogs of Assure)  
 IT Antitumor agents  
 (preclin. antitumor efficacy of quinoxaline analogs of Assure)  
 IT 76578-13-7 76578-16-0 82073-86-7 110945-24-9 157434-99-6, XK 469  
 157435-00-2 157435-13-7 157542-87-5, XB 947 157542-89-7  
 157542-90-0 220935-14-8 220935-15-9  
 220935-16-0 220935-17-1 220935-18-2 220935-20-6

220935-22-8 220935-25-1 220935-27-3

220935-29-5

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study) (preclin. antitumor efficacy of quinoxaline analogs of Assure)

RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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IT 157435-00-2 220935-14-8 220935-15-9

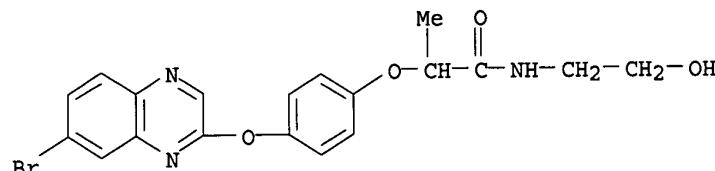
220935-16-0 220935-18-2 220935-22-8

220935-25-1 220935-29-5

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study) (preclin. antitumor efficacy of quinoxaline analogs of Assure)

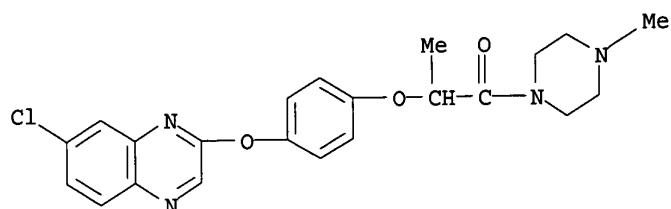
RN 157435-00-2 HCPLUS

CN Propanamide, 2-[4-[(7-bromo-2-quinoxalinyloxy)phenoxy]-N-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)



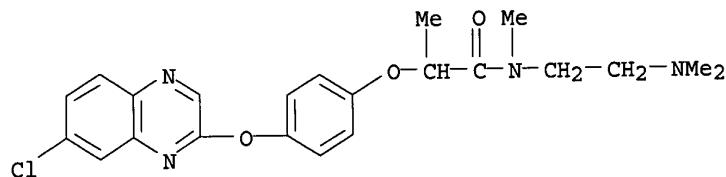
RN 220935-14-8 HCPLUS

CN Piperazine, 1-[2-[4-[(7-chloro-2-quinoxalinyloxy)phenoxy]-1-oxopropyl]-4-methyl- (9CI) (CA INDEX NAME)



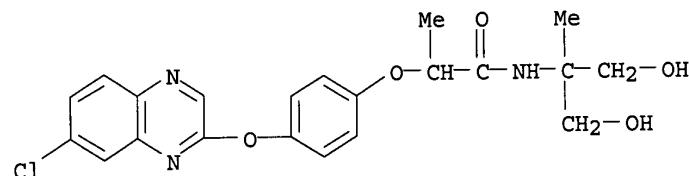
RN 220935-15-9 HCPLUS

CN Propanamide, 2-[4-[(7-chloro-2-quinoxalinyloxy)phenoxy]-N-[2-(dimethylamino)ethyl]-N-methyl- (9CI) (CA INDEX NAME)



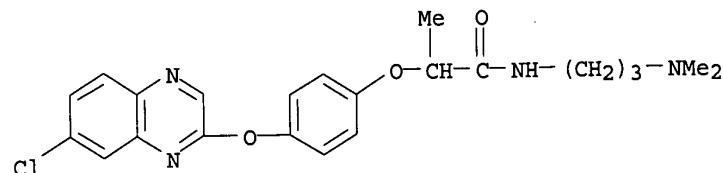
RN 220935-16-0 HCPLUS

CN Propanamide, 2-[4-[(7-chloro-2-quinoxalinyloxy)phenoxy]-N-[2-hydroxy-1-(hydroxymethyl)-1-methylethyl]- (9CI) (CA INDEX NAME)



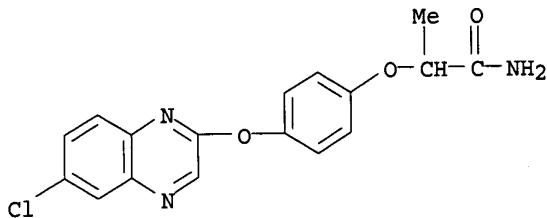
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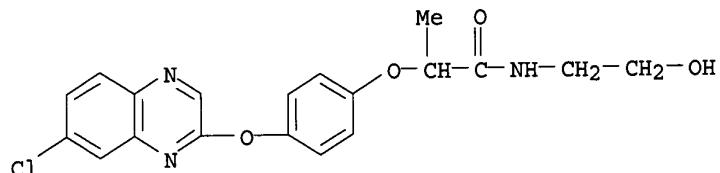


RN 220935-22-8 HCPLUS

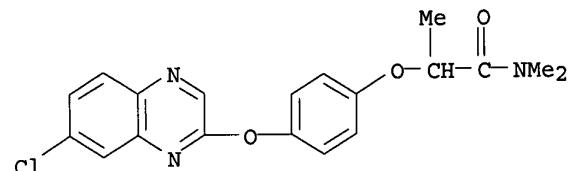
CN Propanamide, 2-[4-[(6-chloro-2-quinoxalinyloxy)phenoxy]- (9CI) (CA INDEX NAME)



RN 220935-25-1 HCPLUS  
 CN Propanamide, 2-[4-[(7-chloro-2-quinoxalinyl)oxy]phenoxy]-N-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)



RN 220935-29-5 HCPLUS  
 CN Propanamide, 2-[4-[(7-chloro-2-quinoxalinyl)oxy]phenoxy]-N,N-dimethyl- (9CI) (CA INDEX NAME)



L28 ANSWER 5 OF 5 HCPLUS COPYRIGHT 2004 ACS on STN  
 AN 1994:557671 HCPLUS  
 DN 121:157671  
 ED Entered STN: 01 Oct 1994  
 TI 2-[(quinoxalinyl)phenoxy]propanoates and related derivatives as  
 anticancer agents  
 IN Behrens, Carl Henry; Dusak, Betsy Ann; Harrison, Barbara Ann; Orwat,  
 Michael James  
 PA Du Pont Merck Pharmaceutical Co., USA  
 SO PCT Int. Appl., 56 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 IC ICM C07D241-44  
 ICS A61K031-495  
 CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI WO 9413647	A1	19940623	WO 1993-US11936	19931214
			W: AU, BR, CA, CZ, FI, HU, JP, KR, NO, NZ, PL, RU, SK	
			RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE	

AU 9456867	A1	19940704	AU 1994-56867	19931214
US 5696119	A	19971209	US 1994-367481	19941228
PRAI US 1992-991525			19921215	
WO 1993-US11936			19931214	

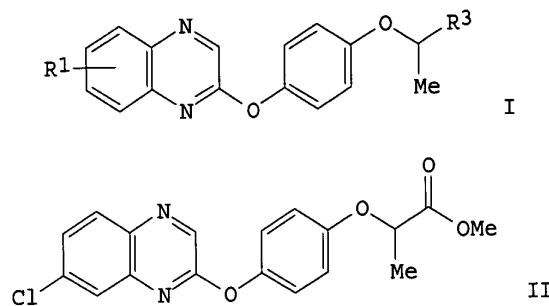
## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
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WO 9413647	ICM	C07D241-44
	ICS	A61K031-495

OS MARPAT 121:157671

GI



AB The title [(2-quinoxalinyloxy)phenoxy]propanoates I (R1 = chloro, bromo; R3 = carboxy, alkoxycarbonyl, amido) were disclosed. The use of I for the treatment of tumors is claimed. Pharmaceutical compns. containing I for the treatment of cancer were described. A prepared example compound is (±)-2-[4-[(7-Chloro-2-quinoxalinyloxy)phenoxy]propanoic acid [ester of (±)-quizalofop] (II).

ST neoplasm inhibitor quinoxalinyloxyphenoxy propanoate prep; quizalofop ester prep neoplasm inhibitor; tumor quinoxalinyloxyphenoxy propanoate prep; cancer quinoxalinyloxyphenoxy propanoate prep

IT Neoplasm inhibitors  
([(quinoxalinyloxy)phenoxy]propanoates)

IT Neoplasm inhibitors  
(leukemia, [(quinoxalinyloxy)phenoxy]propanoates)

IT 78104-71-9P 157435-13-7P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

IT 2427-71-6P, 6-Chloro-2-quinoxalinol 18671-97-1P, 2,6-Dichloroquinoxaline 59489-30-4P, 2(1H)-Quinoxalinone, 7-chloro- 59489-31-5P, Quinoxaline, 2,7-dichloro- 157435-07-9P 157435-08-0P 157435-09-1P 157435-11-5P 157435-12-6P 157542-91-1P 157542-92-2P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as intermediate for [(quinoxalinyloxy)phenoxy]propanoate neoplasm inhibitor)

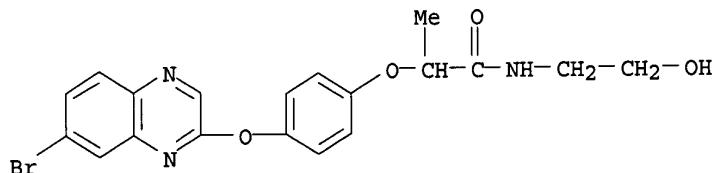
IT 76578-13-7P 76578-49-9P 78104-71-9P, Methyl (±)-2-[4-[(7-Chloro-2-quinoxalinyloxy)phenoxy]propanoate 81466-27-5P 157434-99-6P 157435-00-2P 157435-01-3P 157435-02-4P 157435-03-5P 157435-05-7P 157435-06-8P 157435-10-4P 157542-87-5P, Methyl (R)-2-[4-[(7-Chloro-2-quinoxalinyloxy)phenoxy]propanoate 157542-88-6P, Methyl (S)-2-[4-[(7-Chloro-2-quinoxalinyloxy)phenoxy]propanoate 157542-89-7P, Sodium (R)-2-[4-[(7-Chloro-2-quinoxalinyloxy)phenoxy]propanoate 157542-90-0P, Sodium (S)-2-[4-[(7-Chloro-2-quinoxalinyloxy)phenoxy]propanoate  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of, as neoplasm inhibitor)

IT 95-83-0, 4-Chloro-1,2-phenylenediamine 103-16-2, p-Benzylxyphenol 109-55-7, N,N-Dimethyl-1,3-propanediamine 115-69-5, 2-Amino-2-methyl-1,3-propanediol 141-43-5, reactions 298-12-4 17392-83-5, Methyl (R)-lactate 27871-49-4, Methyl (S)-lactate 67648-61-7, Methyl (±)-2-(4-hydroxyphenoxy)propanoate 89891-65-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reactant for [(quinoxalinyloxy)phenoxy]propanoate neoplasm inhibitor)

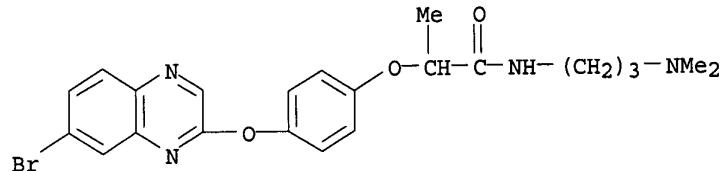
IT 157435-00-2P 157435-01-3P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of, as neoplasm inhibitor)

RN 157435-00-2 HCPLUS

CN Propanamide, 2-[4-[(7-bromo-2-quinoxalinyloxy)phenoxy]-N-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)



RN 157435-01-3 HCPLUS  
 CN Propanamide, 2-[4-[(7-bromo-2-quinoxalinyloxy)phenoxy]-N-[3-(dimethylamino)propyl]- (9CI) (CA INDEX NAME)



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